

Reply to M. Meléndez and W. G. Hoover [arXiv:1206.0188v2]

Michele Campisi,¹ Fei Zhan,² Peter Talkner,¹ and Peter Hänggi¹¹*Institute of Physics, University of Augsburg, Universitätsstr. 1, D-86135 Augsburg, Germany*²*International Center for Quantum Materials, Peking University, 100871, Beijing, China*

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In response to the recent critical comment by M. Meléndez and W. G. Hoover [arXiv:1206.0188v2] on our work [M. Campisi *et al.*, Phys. Rev. Lett. **108**, 250601 (2012)], we show that their molecular dynamics simulations do not disprove our theory but in fact convincingly corroborate it.

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In their comment [1] to our Letter [2], Meléndez and Hoover claim that the Hamiltonian thermostat presented in [2], has “very unusual drawbacks” that “make it impractical for many applications”. In support of this statement they present molecular dynamics simulations. We show here that, quite on the contrary, those simulations corroborate our theory.

For convenience here we reproduce Figure 1 of the comment of Meléndez and Hoover [1], see Fig. 1. The figure shows the numerically computed energy probability distribution of one particle (blue symbols) and two particles (black symbols) in a 1D box interacting with a log-oscillator. In the caption the authors state:

“The blue points correspond to a system of only one thermostated particle, where the results failed to converge to the theoretical prediction during the simulation run.”

Meléndez and Hoover make a mistake in calculating the “theoretical prediction” in the case of one particle. The theory predicts that the probability density function is the Gibbs distribution:

$$\rho(\mathbf{q}, \mathbf{p}) = e^{-H_S(\mathbf{q}, \mathbf{p})/T} / Z(T), \quad (1)$$

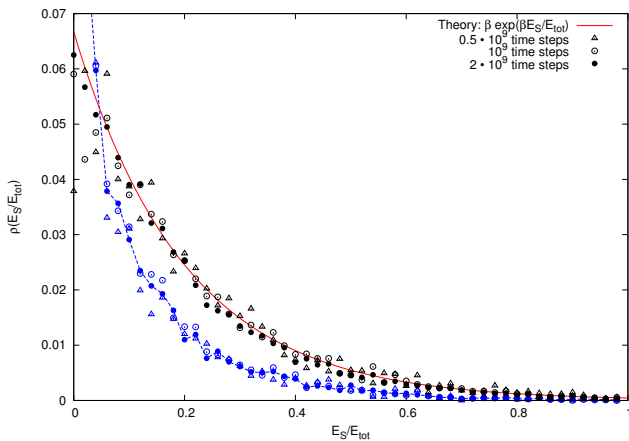


FIG. 1: Figure 1 of the comment of Meléndez and Hoover, Ref. [1]

where $Z(T)$ is the partition function, see Eq. (7) of our Letter. In the energy space the Gibbs distribution function reads, as shown in statistical mechanics textbooks [3], and also mentioned in our Letter [2],

$$\rho(E_S) = \frac{e^{-E_S/T} \Omega_S(E_S)}{Z(T)}, \quad (2)$$

where $\Omega_S(E_S)$ is the density of states of the system. It is well known that the density of states of a system with a Hamiltonian consisting in the sum of n quadratic terms is of the form $\Omega_S(E_S) \propto E_S^{n/2-1}$ [3]. For one particle in a 1D box, $n = 1$, and $\Omega_S(E_S) \propto E_S^{-1/2}$. For two particles in a 1D box, $n = 2$, and $\Omega_S(E_S)$ is a constant, as we explicitly said in our Letter [2]. Therefore the (blue) data in Fig. 1 from a simulation with one particle should be compared with

$$\rho(E_S) = \frac{e^{-E_S/T} E_S^{-1/2}}{\int_0^\infty e^{-E_S/T} E_S^{-1/2} dE_S} \quad (\text{one particle}) \quad (3)$$

and the (black) data in Fig. 1 from a simulation with

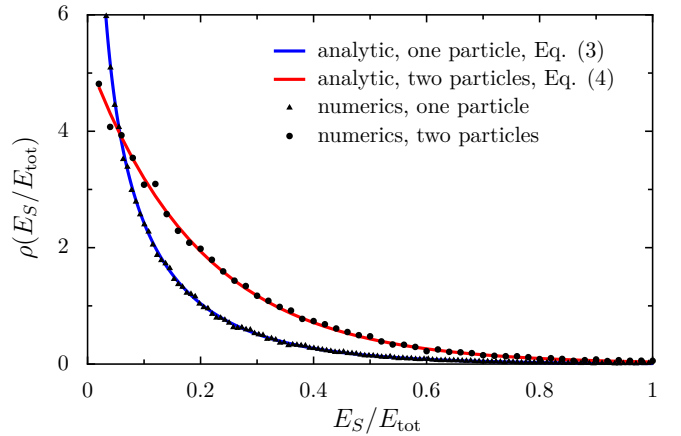


FIG. 2: Our own simulations with one and two thermostated particles in a 1D box, compared with the correct theoretical predictions, Eq. (3) and (4), respectively.

two particles should be compared with

$$\rho(E_S) = \frac{e^{-E_S/T}}{\int_0^\infty e^{-E_S/T} dE_S} \quad (\text{two particles}) \quad (4)$$

that is the red line in Fig. 1.

Meléndez and Hoover mistakenly compare the one-particle data sets with Eq. (4), which pertains instead to the case of two particles only.

Rather than evidencing a “very unusual drawback” of our work, the simulations of Meléndez and Hoover corroborate our theory. See our own simulations in Fig. 2 compared with the correct theoretical predictions, Eqs. (3) and (4) respectively. In comparing our simulations in Fig. 2, with Hoover and Melendez simulations in Fig. 1, note that the main difference is the scale of the vertical axis. This is because, unlike Meléndez and Hoover, we have properly normalized the data so that the area below the curves is 1, as we did in our Letter [2].

In Fig. 2 of their comment [1], Meléndez and Hoover provide the results from a simulation of a 1D chain of eighteen quartic oscillators, which are linearly coupled to two log-oscillators of same strength T . Actually that figure demonstrates a convergence of the particle temperatures toward the value given by the log-oscillators strength T , apparently in agreement with our theory. In

Fig. 3 of their comment [1], Meléndez and Hoover provide the results from a similar simulation but for a nonequilibrium scenario with the two log-oscillators having different strengths T_1 and T_2 . These simulations with linear chains, are neither sufficiently documented, nor conclusive. It is not possible to infer whether the simulations were done in a proper parameter regime and to draw any conclusions from them. The question whether and under which conditions log-oscillators may be employed to simulate non-equilibrium situations is off-topic with respect to the focus of our Letter [2], and needs further thorough investigations.

To sum up, the claim of Meléndez and Hoover that logarithmic oscillators “are not very useful in most practical applications, whether simulations or experiments” has no scientific foundation.

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- [1] M. Meléndez and W. G. Hoover, arXiv:1206.0188v2 (2012).
 - [2] M. Campisi, F. Zhan, P. Talkner, and P. Hänggi, Phys. Rev. Lett. **108**, 250601 (2012).
 - [3] K. Huang, *Statistical Mechanics*, 2nd Ed. (Wiley, New York, 1987).